Freshwater Quality Monitoring Protocol
San Francisco Area Network

Standard Operating Procedure (SOP) # 10

DATA ANALYSIS

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Prev. Version #	Revision Date	Author	Changes Made	Reason for Change	New Version #
1.0	8/5/05	M. Cooprider	Additional guidance on data analysis and presentation	Preparation for formal peer review	1.01

Only changes in this SOP will be logged. "Version numbers increase incrementally by hundredths (e.g. version 1.01, version 1.02, …etc) for minor changes. Major revisions should be designated with the next whole number (e.g., version 2.0, 3.0, 4.0 …). Record the previous version number, date of revision, author of the revision, identify paragraphs and pages where changes are made, and the reason for making the changes along with the new version number" (Peitz et al, 2002).

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1.0 INTRODUCTION AND ACKNOWLEDGEMENTS

Water quality data typically has a non-normal distribution due to a lower bound of zero, the presence of outliers, and positive skewness. Seasonality and autocorrelation are also common as well as covariance with other variables such as discharge (Helsel and Hirsch, 2002). Water quality data is usually highly variable, both temporally and spatially. Data characteristics often utilized for water quality data include: a measure of the center of the data, a measure of spread or variability, a measure of the symmetry of data distribution, and possibly estimates of extremes (Helsel and Hirsch, 1992). This SOP provides guidance on how to prepare and analyze data given these characteristics. Sections of this SOP were obtained from the Greater Yellowstone Network SOP#9 - Data Analysis Procedures in the *Regulatory Water Quality Monitoring Protocol* (O'Ney, 2004). David Lewis (University of California Cooperative Extension) also provided valuable insight. Finally, the internet accessible text, *Statistical Methods in Water Resources* (Helsel and Hirsch, 1992) was frequently consulted. While the basics of water quality data analysis are covered here, this statistics text should be followed for greater details.

2.0 PREPARING THE RAW DATA SET FOR ANALYSIS

2.1 Censored Data and Outliers

Water quality data is often "censored" or reported as less than the detection limit. In some cases, there are also instances of data values greater than or equal to the upper detection limit. This occurs most frequently with fecal coliform data since the proper dilution, based on the expected range, is sometimes difficult to predict particularly during storm events. Censored data is considered outside the range of quantitation (i.e., it cannot be quantified and a number cannot be assigned to it) and generally should not be statistically analyzed. However, censored data are presented as less than or greater than the ML in order to compare it to water quality criteria (Irwin, 2004). Therefore, although these data should not be included in statistical analysis, they are still useful for water quality assessment.

More advanced methods for dealing with censored data are outlined in Ch. 13 in Helsel and Hirsch (1992). This chapter describes how observed data may be combined with censored data in order to calculate estimates of summary statistics. Also refer to the recent publication *Nondetects and Data Analysis: Statistics for Censored Environmental Data* (Helsel, 2004).

The SFAN Quality Assurance Project Plan (SOP#4) describes the details of data quality objectives and measurement quality objectives in relation to data reporting. A summary of how data should be reported is as follows:

- Values below the Method Detection Limit (MDL) are to be reported as a (<) sign followed by the actual MDL value, and flagged with a ND = not detected.
- Values between the MDL and the ML (or quantification limit) should be reported as the actual measured value, with a flag that is carried all the way through data storage, handling, and reporting. The flag is DNQ = detected, not quantifiable. These data are considered semi-quantitative.
- Values above the ML (or quantification limit) are deemed as acceptable values without reservation, and are shown as the actual measured value, and assigned a QA code of A (acceptable without reservation).

Do not immediately remove outliers from a data set because they appear unusual. It is important to first verify that no human errors have been made such as copying a number wrong or putting a decimal point in the wrong place. Rather than eliminating possibly important data in order to use standard statistical analyses (e.g., tests requiring normally distributed data), methods that are resistant to outliers should be utilized. (Helsel and Hirsch, 1992). Some of the summary statistics that are resistant to outliers are discussed in Section 3.0 of this SOP.

2.2 Replicates and Data Transformations

Replicates should be averaged together and the single mean value used in their place for analysis, or the median value may be used. The standard deviation or range of the replicates provides an estimate of the variability in the measurement technique (Stafford and Horne, 2004).

The goal of data transformations is to "make data more symmetric, to make data more linear, and to make data more constant in variance" (Helsel and Hirsch, 2002). Some examples include logarithmic transformations and adjusting data for flow. Use logarithmic transformations with fecal indicator bacteria (FIB) data since transforming allows for a more simple data analysis and graphical display of data with a range that often spans over several orders of magnitude. Log transformations are also commonly used with discharge measurements and sometimes with nutrient data. Basically, use log transformations on data when there is a broad range of data. It is helpful to display both the transformed data and non-transformed data to understand how transformations affect the data. This is particularly useful when presenting to a general audience (Dave Lewis, personal communication, 29 July 2005).

Flow adjusted or flow-weighted data is simply the concentration (C) of the analyte divided by the discharge (Q). Transformations (either logarithmic or flow-adjusted) can make the data more "normal" (symmetric) and increase the possibility of using parametric statistics which are slightly more powerful at determining statistical differences. Transforming the data does not change the median and interquartile range (IQR). However, transforming does change the mean and standard deviation (Helsel and Hirsch, 1992). This is why both the mean and standard deviation as well as the median and IQR are reported for water quality data or any other data that is typically non-parametric.

3.0 DATA ANALYSIS

Before data analysis:

- Review data promptly to detect potential outliers or errors
- Conduct log transformations on bacteria data and calculate flow-weighted data
- Use the mean of replicate samples for statistical analysis
- Don't conduct statistical analyses on censored data but use all data for overall comparisons against water quality criteria.
- Export data from the NPSTORET to Microsoft Excel to conduct analysis. Further analysis can be conducted with other statistical software. However, NPSTORET does have several statistical and graphical functions that could be used as they become available.

Use graphs before data analysis to learn more about the data set. A plot of raw data values (for one site) against time is an important preliminary tool to assist in visualizing the data distribution and to provide a check for temporal patterns and extreme values (outliers).

3.1 Summary Statistics and Tabular Data Presentation

The following descriptive statistics should be performed:

Mean
Standard Error
Median
Std. deviation
Variance
Kurtosis (peakedness)
Skewness (lack of symmetry about the mean)
Range/Interquartile Range (IQR)
Minimum
Maximum
Sum
Count
Confidence intervals for mean and median (95 or 99% confidence level)

- Use all data (including censored data) for comparison against water quality criteria.
- Analyze reference or control sites separately to determine a baseline for specific streams.
- To limit seasonal variability, conduct statistical tests on each of the different seasons.
- Summarize data for each site and for each parameter seasonally and annually
- Summarize data from all stations within each watershed seasonally and annually.
- Compare data from stations upstream and downstream of a suspected pollution source or tributary.
- Use flow (discharge) weighted data and group data by season to account for seasonal variation.
- Discrete and continuous data should be analyzed separately. However, data from the same days may be compared for quality control and to obtain a relationship between the datalogger readings and instantaneous monthly/weekly data.
- Determine the inherent variability of a sampling technique by calculating the standard deviation of replicates (see as Section 3.1.2 below)

• Present data in tabular form for each station and watershed as follows:

SFAN I&M Water Year 2006 Water Quality Data - Station ID

Date	pH	TEMP	DO	COND	Total NH3	*NH3-tox*	NO3	Total N	FC	TURB
_ Nov 06										
_ Dec. 06										
_ Jan 06										
_Feb 06										
_March 06										
_April 06										
_May 06										
_June 06										
_July 06										
_Aug 06										
_Sept 06										
_Oct 06										
Statistics										
Mean										
Std. Error										
Median										
Std. Dev.										
Variance										
Kurtosis										
Skewness										
Range										
Min										
Max										
Sum										
Count										
Confidence Level										

- Next, summarize all data and compare to water quality criteria using the following example (from Rugg, 2000).

Table I
All 99-2000 (98-9) Data

	Dissolved Oxygen mg/l	Total Ammonia mg/l	Un-ionized Ammonia mg/l	Conductivity - mhos/cm
Average *	**9.29** (10.09)	**0.420** (1.004)	**0.0068** (0.014)	**577** (412)
Range	**6.2-10.3** (2.0-15.9)	**0-25.2** (0-17.4)	**0-1.071** (0- 0.377)	**8-2342** (75-1690)
Criteria**	5.0-7.0	-	0.025	750
Exceedances	**53** (14)	-	**39** (77)	**125** (73)
Percent Exceedance	**6.36** (2)	-	**4.68** (12)	**15** (12)

* 833 measurements
** SF Bay RWQCB Basin Plan

3.1.1 Statistics for fecal coliform data

In addition to the above summary statistics, a geometric mean should be calculated for fecal coliform and *E. coli* data.

For the Olema Creek data (Pathogen TMDL sampling), calculate the 30-day geometric mean of samples from five consecutive weeks to determine whether standards are being exceeded. Water quality standards are listed in SOP#6 and in the Protocol Narrative. To calculate the estimated geometric mean (*In* O'Ney, 2005; adapted from WY-DEQ 1999):

1. convert each CFU count/100ml to its log
2. add the logs
3. divide the total of the logs by the number of samples to get the mean
4. take the antilog of (3); that number is the geometric mean (in CFU/100mL)

Example: test results are 760, 3100, 300, 632 and 805
Arithmetic mean = 760 + 3100 + 300 + 632 + 805 = 5597 / 5 = 1119.4
Arithmetic median = 760
Geometric mean = 816.58

$\log_{10}$ 760 = 2.88
$\log_{10}$ 3100 = 3.49
$\log_{10}$ 300 = 2.48

$\log_{10}$ 632 = 2.80
$\log_{10}$ 805 = 2.91
sum of the logs = 14.56
mean of the logs = 14.56/5= 2.912
antilog 2.912 = 816.58

An alternative method is to multiply the CFU counts/100ml together and take the nth root, where n = number of samples (5 in this example). Using the test results above:

760 x 3100 x 300 x 632 x 805 = 3.6 x 1014
(3.6 x 1014)1/5 or (3.6 x 1014).2 = 815.19

Results from field blanks should also be reviewed to establish that a sample is not being contaminated by conditions associated with the collection or custody of a sample or by cross-contamination during sampling or shipping. Another way to determine whether field methods are adequate is to calculate precision from duplicates. Fecal coliform duplicate precision is calculated for the Number of Colonies /100 ml value (not the log transformation) and is typically set at ±50% . See section 3.2 in this document for guidance on calculating precision.

3.1.2 Calculating Precision

The following is an explanation for calculating precision of field duplicates. Other QA/QC measures, including calculating precision of lab duplicates, are discussed in SOP #4.

(*In* O'Ney, 2004; Adapted from WY-DEQ, 2000)

> Precision is defined as how closely repeated measurements agree with each other. Precision indicates the degree of agreement between sequential independent samples at a site, collected by applying the same collection method. If the sample is representative and the sampling methods are consistent, two or more measurements made consecutively with a field instrument usually agree very closely (less than 10 per cent difference). Estimates of precision are also known as sampling error. Precision should be calculated as soon as results from duplicate analyses are available, no later than 7 days after receipt from laboratory.
>
> The precision measurement is calculated using the relative percent difference (RPD) between duplicate sample results per analyte (parameter). For duplicate samples, the smaller test result is subtracted from the larger test result. The resulting difference is divided by the average of the two results, and the result is multiplied by 100 to express the number as a percent. The formula is: [(S1 - S2) / ((S1 + S2)/2)] x 100 = RPD, where S1 is the larger test result value.
>
> For precision results, not only should RPDs be reported, but also raw numbers. This will allow for calculation of uncertainty statistics later, should this be needed.

3.2 Graphical Data Presentation

Important graphical features or comparisons to utilize include:

- Location (line) showing detection limit on graph
- Distance from suspected source or distance from source
- Display pH, D.O., and temperature on one chart to show relationships
- Parameter against time (shows seasonal changes) for each station
- Parameter against time for all stations in a watershed
- Site comparisons for each parameter
- Display all data for one station on one page
- For continuous data, graph daily, monthly, and seasonally
- Relationships of conductivity to fecal coliforms
- Relationship of flow to all other variables

Chapter 2 (Graphical Data Analysis) and Chapter 16 (Presentation Graphics) of *Statistical Methods in Water Resources* (Helsel and Hirsch, 1992) should be followed for graphical data analysis. Tables can be used in association with graphs but presentation of data should not rely solely on tables. Graphics should generally include:

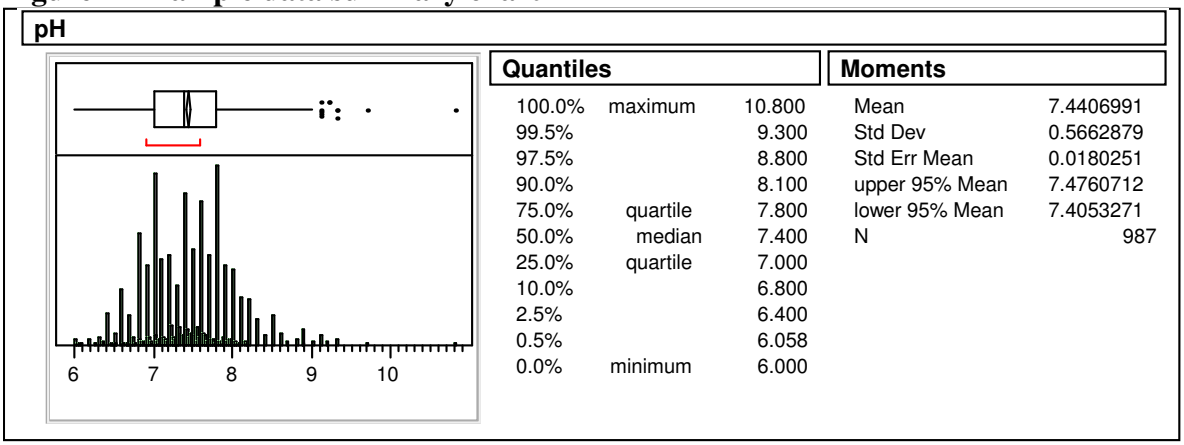
1) **histograms** (e.g., streamflow vs. number of occurrences): useful for depicting large differences in shape or symmetry. They are better for data that have natural categories or groupings ; they are not as good with continuous data since it is difficult to depict this type of data accurately in a discrete group. It would work well for the number of sites exceeding different levels of water quality criteria (e.g., non-contact recreation and contact recreation).

2) **simple box plots** (box and whiskers plot) Whiskers are drawn to the points of maximum and minimum data, a box depicting the 25^{th} and 75^{th} percentile is drawn, and a horizontal line through the box depicts the median. These can be used for reviewing one set of data or for comparing multiple data sets. "They are valuable guides in determining whether central values, spread, and symmetry differ among groups of data." They can be used to determine whether tests based on the assumption of normality can be used (Helsel and Hirsch, 1992).

3) **scatterplots** – relationship between two variables (e.g., flow vs. fecal coliforms); a "smoothe" may be used to help determine the relationship of x to y. The preferred procedure for this is LOWESS (LOcally WEighted Scatterplot Smoothing) (Helsel and Hirsch, 1992).

Summary tables, histographs, and box and whisker plots can be used to show median and interquartile ranges (non-parametric), mean and standard deviation (parametric), and 95% confidence intervals for means and medians. Example histograms and box plots are illustrated in Figures 1 and 2, respectively (from Stafford and Horne, 2004).

Figure 1 Example data summary chart

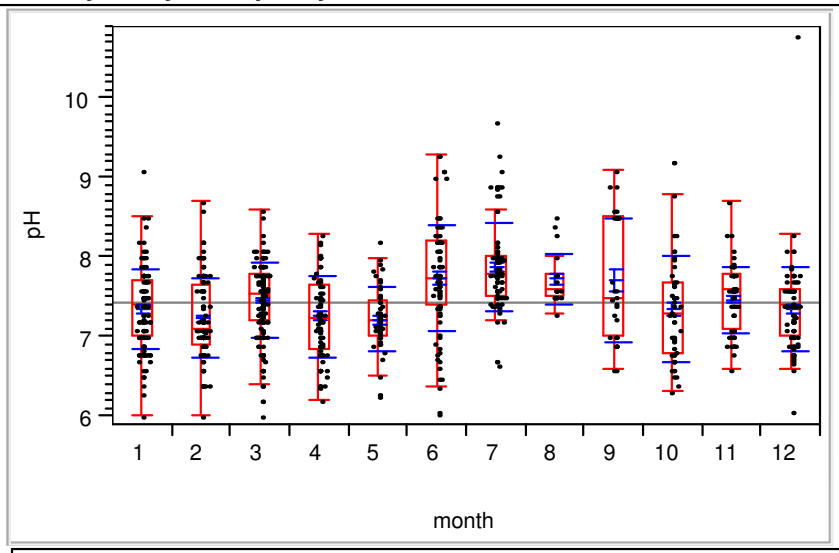


The heights of the bars in the histogram represent the number of times an observation was recorded. The outlier box-plot above the histogram shows the interquartile range within the box. The line across the middle of the box identifies the median sample value. The diamond represents the mean and 95% confidence interval. The lines extending from each end of the box, or the whiskers, encompass the quartiles +/- 1.5x (interquartile range). Points beyond the whiskers indicate extreme values that are possible outliers. The bracket along the edge of the box identifies the shortest half, or the densest 50% of the observations. To the right of the histogram, the quantiles and moments are displayed. The total number of observations is listed as N.

from Stafford and Horne, 2004

Figure 2. Example box and whiskers plot, quantiles, and mean and standard deviation summaries by month

Oneway Analysis of pH By month



Quantiles

Level	Minimum	10%	25%	Median	75%	90%	Maximum
1	6	6.8	7	7.4	7.7	8	9.1
2	6	6.74	6.9	7.1	7.65	7.9	8.7
3	6	6.8	7.2	7.53	7.8	8	8.6
4	6.2	6.6	6.8525	7.225	7.64	8	8.3
5	6.25	6.776	7	7.2	7.45	7.824	8.2
6	6.03	6.793	7.4	7.725	8.2	8.5	9.3
7	6.65	7.4	7.5	7.8	8.015	8.888	9.7
8	7.3	7.5	7.5	7.6	7.8	8.38	8.5
9	6.6	6.9	7	7.495	8.5	8.87	9.1
10	6.31	6.6	6.8	7.3	7.685	8.22	9.2
11	6.6	6.9	7.1	7.6	7.8	7.9	8.7
12	6.06	6.824	7	7.39	7.6	7.8	10.8

Means and Std Deviations

Level	Number	Mean	Std Dev	Std Err Mean	Lower 95%	Upper 95%
1	117	7.34658	0.504041	0.04660	7.2543	7.4389
2	133	7.22684	0.494876	0.04291	7.1420	7.3117
3	165	7.45412	0.473718	0.03688	7.3813	7.5269
4	80	7.25337	0.514993	0.05758	7.1388	7.3680
5	53	7.21811	0.409939	0.05631	7.1051	7.3311
6	88	7.73273	0.677939	0.07227	7.5891	7.8764
7	85	7.87094	0.559012	0.06063	7.7504	7.9915
8	21	7.72381	0.320788	0.07000	7.5778	7.8698
9	30	7.70433	0.785821	0.14347	7.4109	7.9978
10	53	7.34094	0.665173	0.09137	7.1576	7.5243
11	69	7.46609	0.415367	0.05000	7.3663	7.5659
12	93	7.34860	0.531717	0.05514	7.2391	7.4581

from Stafford and Horne, 2004

In the example in Figure 2, data from all stations is grouped together for each month. "Level" is referring to month. One drawback of using maximum and minimum values is that as the data set grows, the most extreme values just keep extending and don't necessarily reflect common

conditions. They are useful for immediate management decisions, since they often indicate something is wrong, but are not as useful for an overall sense of the water quality conditions.

3.3 Long-term trend analysis

Long-term trend analysis is generally conducted on five to ten years of data more. However, data for most SFAN watersheds will be collected on two-year intervals. Trend analysis can be conducted on 4, 6, and 8 years of data and so on. The basic question in trend detection is "What is the affect of time on the given parameters?" If time is shown to have an affect, then we to ask "Are changes sudden or gradual?" and "What is the extent of the change?" Trend analysis should account for flow in order to be meaningful. Trend analysis should also account for seasonal differences. The ability to detect trends is dependent upon the variability of the data, as well as the responsiveness of the indicators (parameters), and sample size (Irwin, 2004).

3.3.1 Basic trend analysis: Graphing and other useful tools

For trend analysis, at a minimum, produce histograms displaying data from multiple years. Combine all data from all stations and display the maximums, means, range and number of water quality criteria exceedences (if applicable). Use the following graphs from Rugg (2000) as a guide.

Figure 5
All Data-Maximum Total NH3

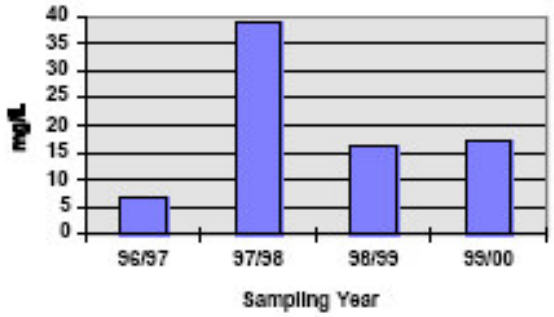
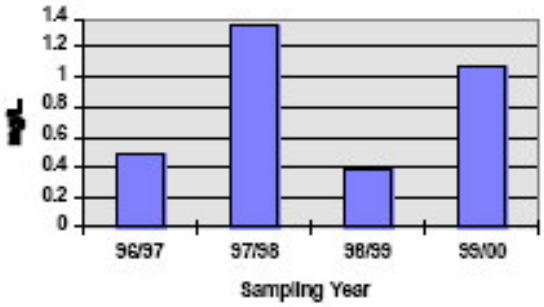


Figure 6
All Data-Maxumum Toxic NH3



When graphing data for more than one year, seasonal patterns may be readily apparent. Each seasonal effect (strata) should be partitioned and graphed alone such that trends that develop over the long-term become visually clear. Examples of partitioned graphic representations are:

- the concentration of a particular variable (y-axis) during low-flow periods (x-axis),
- suspended sediments during winter storm events (refer to stream hydrograph),
- nutrient values during the spring and summer (high productivity)
- dissolved oxygen during peak temperature periods (summer)

Tips:
- If the same data is used for long-term trends and short-term exceedences measured values can be averaged over each quarter, so that there is just one value per quarter.
- The above approach can also be used for analysis of large (past) data sets with varying sampling frequencies

Maps displaying water quality trends are also a useful tool. Water quality stations can be identified by an increasing or decreasing trend or no trend. Another possibility is to utilize (or create) a water quality index to present SFAN data to a wide audience. One good example of a WQI was developed by the Washington Department of Ecology (Hallock, 2002).

3.3.2 Trend Detection *(modified from Hirsch et al., 1991)*

Other routine trend analyses can be done according to Helsel's Internet Published Text Book (Helsel and Hirsch 1992). Consult Ch. 12 of the Helsel and Hirsch (1992) text for techniques for trend analysis. This includes accounting for the affect of flow, other seasonal affects, and addresses both parametric and nonparametric statistics. Stafford and Horne (2004), suggest the use of monotonic trends to look for gradual changes in water quality. The protocol narrative also discusses various data analysis scenarious based on the distribution of the data (parametric, non-parametric, or mixed) and whether the data is flow-weighted. The Helsel and Hirsch (1992) text covers this in greater detail.

Tables 1 through 4 summarize recommendations for monotonic and step trend detection, depending on the type of data under analysis. Monotonic trends are to be used for gradual changes, and step trends are to be used before and after a change at a specific point in time. The monotonic trend hypothesis is more commonly used for general monitoring unless there is a reason to test for a step trend. The step trend hypothesis may be used after implementation of best management practice if there is expected to be a detectable change. The parameters classified as "mixed" in the first two tables have both parametric and nonparametric components that are typically executed in separate steps.

Regression on season uses a periodic function of time of year, as does Tobit regression on season. Tobit regression is a type of linear regression that considers both censored and non-censored values of the response variable, and uses maximum-likelihood estimation for determining slope and intercept of the modeled trend line (Hoppe, 2003).

Deseasonalizing is done by subtracting seasonal medians from each of the values to be regressed. The Seasonal Kendall test is the Mann-Kendall test for trend done for each season, with the Seasonal Kendall test statistic being the sum of the several Mann-Kendall test statistics. The seasonal Kendall trend test accounts for seasonal variations in concentrations by comparing ranks of data from the same recurring time intervals; for example, in a four-season year, springtime values are compared only to other springtime values, summer values to summer values, and so forth.

LOWESS is locally weighted scatterplot smoothing. The LOWESS curve represents a nonlinear, smoothed relation between two variables (instantaneous discharge and each water quality parameter). The method uses a series of weighted least squares regressions; observations are weighted by both distance from the fitted line and the magnitude of residuals from the previous regression. LOWESS is more desirable than simple regression because it makes no assumptions of data linearity or normality (Hoppe, 2003). Flow may be replaced by a transformation of flow in any of these analyses.

The Seasonal Rank Sum test is the Rank Sum test (also known as the Mann-Whitney "U" test (Kirchner, 2003), done for each season, with the Seasonal Rank Sum test statistic being the sum of the several test statistics.

Table 1

Options for testing monotonic trends in uncensored water quality data		
	Not Flow Adjusted	Flow Adjusted
Fully parametric	Regressions of concentration on time and season	Regression of concentration on time, season, and flow
Mixed	Regression of deseasonalized concentration on time	Seasonal Kendall on residuals from regression of concentration on flow
Nonparametric	Seasonal Kendall	Seasonal Kendall on residuals from LOWESS of concentration on flow

Table 2

Options for testing step trends in uncensored water quality data		
	Not Flow Adjusted	Flow Adjusted
Fully parametric	Analysis of covariance of concentration on season and group (before and after)	Analysis of covariance concentration on season, flow and group
Mixed	Two-sample t test on deseasonalized concentration	Seasonal Rank Sum on residuals from regression of concentration on flow
Nonparametric	Seasonal Rank Sum	Seasonal Rank Sum on residuals from LOWESS of concentration on flow

Table 3

Options for testing for monotonic trends in censored water quality data		
	Not Flow Adjusted	Flow Adjusted
Fully parametric	TOBIT regression of concentration on time and season	TOBIT regression of concentration on time, season and flow
Nonparametric	Seasonal Kendall	no test available

Table 4

Options for testing for step trends in censored water quality data		
	Not Flow Adjusted	Flow Adjusted
Fully parametric	TOBIT analysis of covariance of concentration on season and group	TOBIT analysis of variance of concentration on season, flow and group
Nonparametric	Seasonal Rank Sum	no test available

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